Electronic Bands Behaviour at Sinusoidal Potential Presence of Incommensurate Crystals

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Abstract

On the basis of solving the Schrodinger and Mathieu equations, for the case of crystal field perturbed by one-dimensional sinusoidal potential of the modulated phase in uniaxial ferroelectrics, it has been shown that the positions of electronic levels are sensitive to the ratio of periods of the crystal field and the perturbation potential. Considering the energy states as prototypes of bands normalized by perturbation, one can come to the conclusion that the level of the states is the same as in the initial lattice, when the commensurate perturbation period is doubled. Incommensurate changes in the modulation parameter are shown to lead to modification of the distance between the energy levels or bands.

Key words: incommensurate structures, electronic spectra

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Introduction

It has been shown in the middle of 1970s [1] that a quantization of electron and hole levels occurs for thin, quantum-size layers in semiconductors, which differ by the bandgap energy. In this case, a carrier is confined to a narrow bandgap well by larger bandgap barrier layers. Therefore, the semiconductor material in which these layers are constructed may be considered as a medium with the quantum wells. Such superlattice structures possess a number of advantages when applying them in optoelectronics, in comparison with bulk materials. For example, the electro-absorption coefficients in multiple quantum-well structures are approximately 50 times larger than that for the bulk semiconductors [2], due to a quantum confining Stark effect [3]. Such a large value of electro-absorption coefficients follows from exciton confinement by the quantum well. The usage of electro-absorption effect in quantum-well materials for direct light modulation leads also to the other benefits such as increasing modulation rates up to 20Gbit/s [4] and broadening the bandwidths towards GHz range [5]. The similar advantages achieved with application of tre quantum-well devices (e.g., the electrooptic switches) are based on electro-absorption effect [6].

Besides, a principal problem of quantum-size effects application is a difficulty of preparation of quantum-well structures. Such thin layers are usually constructed with the molecular beam epitaxy (MBE) or the metal organic chemical vapour deposition (MOCVD) techniques. The above techniques enable one to prepare controllable layers with a thickness less than 100 Å [7]. On the other hand, those methods are expensive and need a lattice

matching. In addition, MOCVD requires a high-level industrial safety because the metal-organic gases are extremely toxic and the carrier gas dangerously explosive.

On the other side, it is known that the modulated superlattice structures exist also in incommensurate (IC) phases of dielectric and semiconductor crystals [8]. The IC structures usually occur in the temperature range between the ordered (ferroelectric or ferroelasic) and disordered (paraelectric or paraelastic) phases [9]. The direct X-ray, neutron scattering, electronic microscopy and the atomic force microscopy measurements suggest the existence of superlattice in the IC phases. The period, amplitude and shape of the modulation wave change with temperature. In the vicinity of the phase transition from paraelectric or paraelastic phase to the IC phase, the shape of the modulation wave is close to sinusoidal, whereas near the phase transition to the ordered phase it approaches to the square waveform. The periods of the order parameter modulation in different crystals are within the limit of tens of the lattice parameter dimension or somewhat larger. If, for example, the spontaneous electric polarization plays a role of the order parameter, then, probably, the bandgap should be also modulated due to the known Franz-Keldysh effect. In such a case, the probability of quantum confinement in the well would depend on the dimension of this well, the thickness of the barrier and the depth of the well. It means that there are all reasons for supposing that the natural quantum wells in the IC semiconductors should possess the same quantum confinement properties as those in the epitaxy-grown layers.

The present paper is devoted to analysis of electronic spectrum in the crystalline structures with accounting for the modulated IC potential presence.

Theoretical Approach

Let us follow from the electronic potential that may be presented in the form of two terms with different periodicity, including the case when the periodicity is IC.

The objects of our study are ferroelectric crystals, whose initial structure exists at some conditions that could be distorted or modified with a periodic field of electric dipoles, i.e. with a potential additional to that of the crystal field. This additional potential may be either commensurate or IC, with respect to the crystal field potential. Let us analyse the effect of degree of incommensurability on the electronic spectrum of ferroelectrics. We restrict the consideration to a one-dimensional model. Although this cannot be realized in nature, the model can provide qualitative conclusions valid as a quite reasonable approximation for the two- or three-dimensional objects. Besides, the one-dimensional character is peculiar for the polarization and the additional potential that modifies the crystal field in case of uniaxial ferroelectrics. The other important fact is that the amplitude of the additional potential is much smaller than that of the crystal field. Taking into account the sinusoidal profile of the modulation wave near the phase transition temperature from the normal to the IC phase, one can use the perturbation theory for solving the problem. With decreasing temperature, the profile approaches the square waveform, but the additional satellites usually possess a comparatively small intensity. Thus, we shall consider only a sinusoidal modulation.

Let the one-dimensionally periodic potential is described with the dependence $\sim \cos 2z$. Then the steady-state Schrodinger equation can be written in the form of Mathieu equation:

$$\frac{\partial^2 \psi}{\partial x^2} + (a - 2q\cos 2z)\psi = 0 . \qquad (1)$$

In Eq. (1) the notations $\frac{2mU(z)}{\hbar^2} = 2q\cos 2z$ and $a = \frac{2mE}{\hbar^2}$ are used, with q being the potential amplitude. If we consider z variable as a coordinate, the analogue

of the cosine argument in the crystalline structure would be kz, where $k=\frac{2\pi}{Na}n$ is the reciprocal lattice vector (a meaning the lattice parameter, Na the basic region of the crystal and $n\in 0...(N-1)$). Below we shall consider the range $z\in[0,\pi]$ that corresponds to na in the lattice parameter units.

The solutions of the Mathieu equation are well known (see, e.g., [10]) and they can be periodic with the periods π or 2π and even or odd. The eigenvalues a_r are $ce_r(z,q)$ and b_r ($se_r(z,q)$) respectively for the even and odd eigenfunctions. Let us analyse the first corrections to the fundamental energy state (a_0) and the first and second excited-energy states (a_1, a_2) caused by the perturbation:

$$\widehat{H}=2Q\cos(2pz), \tag{2}$$

where $p=1/m$ and m is the modulation parameter. The periodic potential is commensurate with respect to the main crystal field for integer p and IC for non-integer p. In framework of the perturbation theory, Q should satisfy the condition $Q\ll q$ and the first correction to the energy of r th state equals to

$$\Delta E_r=\left\langle ce_r\left|\hat{H}\right|ce_r\right\rangle \tag{3}$$

For the small values of q, $ce_r(z,q)$ may be represented with a convergent power series [10]. For the states r=0, r=1 and r=2 this can be written as

$$ce_0(z,q)=\frac{1}{\sqrt{2}}\left[1-\frac{q}{2}\cos 2z+q^2\left(\frac{\cos 4z}{32}-\frac{1}{16}\right)-q^3\left(\frac{\cos 6z}{1152}-\frac{11\cos 2z}{128}\right)+...\right], \tag{4}$$

$$ce_1(z,q)=\cos z-\frac{q}{8}\cos 3z+q^2\left(\frac{\cos 5z}{192}-\frac{\cos 3z}{64}-\frac{\cos z}{128}\right)-q^3\left(\frac{\cos 7z}{9216}-\frac{\cos 5z}{1152}-\frac{\cos 3z}{3072}+\frac{\cos z}{512}\right)+... \tag{5}$$

$$ce_2(z)=\cos 2z-q\left(\frac{\cos 4z}{12}-\frac{1}{4}\right)+q^2\left(\frac{\cos 6z}{384}-\frac{19\cos 2z}{288}\right)+... . \tag{6}$$

For the larger values of q, the series become less convergent. Besides, a comparison of ΔE_0, ΔE_1 and ΔE_2 for the q parameter values q=0.01 (more accurate) and q=0.05 (less accurate) shows the same qualitative behaviour of the energy states (see Figure 1).

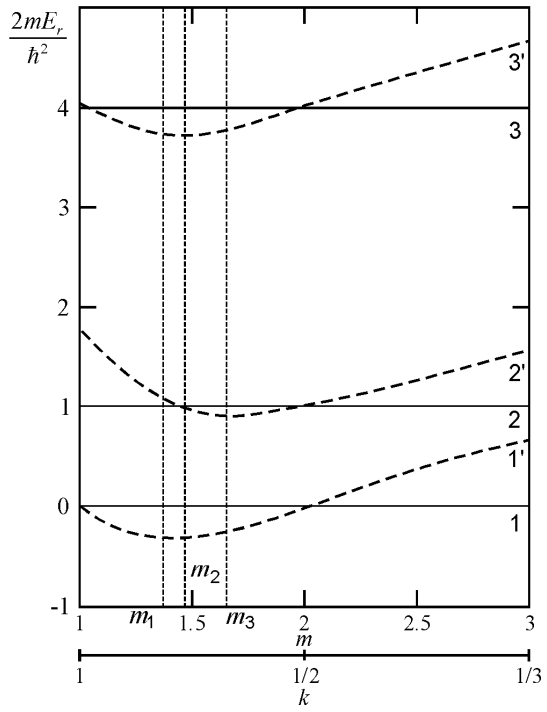

Fig. 1. Schematic dependence of the normalized energy (taken with the accuracy up to the factor $\hbar^2/2m$) of the three lowest states on the modulation parameter m and the k vector of the Brillouin zone (curve 1 corresponds to the energy of the fundamental state E_{00}, 1′ the energy of the modified fundamental state E_0; 2 and 3 the energies of the excited states E_{11} and E_{22}, and 2′ and 3′ the energies of the modified excited states E_1 and E_2).

Results and discussion

The dependences of the energy states and the states modified by the perturbation upon the modulation parameter are presented in Figure 1. According to [10], we have E_0=-5×10^{-5}, E_1=0.99 and E_2=4.00 at q=0.01. The ΔE_r value is calculated in the units of Q/10. It is seen that the energies of the non-perturbed fundamental state and the excited states do not depend on the m parameter. However, the energy of the fundamental state perturbed by the IC modulation field already essentially on the modulation parameter.

Two special points are observed on these dependences: a minimum of energy that corresponds to the modulation parameter value m≈1.35 and a point of equality of energies of the non-perturbed and perturbed fundamental states that corresponds to doubling of the unit cell. It is interesting to note that the minimum of the fundamental electronic level energy may correspond to some intermediate, IC value of the lattice modulation parameter. It means that, from the point of view of the electronic structure, the IC state may become energy-equilibrium and so preferable one under certain conditions. The m-dependence of the perturbed excited state E_1 exhibits three special points. One of them corresponds to a minimum of the energy appearing at m≈1.7, while the two other – to equality of the energies of the perturbed and non-perturbed levels at m≈1.45 and m≈2. One can see that the equality of energies of the perturbed and non-perturbed states at the doubled unit cell is peculiar to all of the considered states. The m-dependence of the excited perturbed energy state E_2 also manifests a minimum, but at the m-parameter value ~1.5.

On the other side, it seems to be possible to consider the energy levels as prototypes of the energy bands, the valence and the conduction bands. In such a case, the distance between these bands may be regarded as a bandgap. For example, consider E_0 as the prototype of the valence band and E_1 as that of the conduction band. Then the increase in the modulation parameter within the range of $[m_1, m_3]$ leads to decreasing distance between them (i.e., the bandgap value). When E_1 and E_2 are regarded as the prototypes of the valence and conduction bands, the increase of m in the range of $[m_1, m_2]$ induces the inverse effect of increasing bandgap width.

Conclusions

The Schrodinger and Mathieu equations are solved for the case of crystal field perturbed by the one-dimensional sinusoidal potential of the modulated phases occurring in the uniaxial ferroelectrics. It is shown on this basis that the positions of electronic levels are sensitive to the ratio of periods of the crystal field and the perturbation potential. The dependence of the perturbed fundamental and the excited-energy levels possess the common peculiarities. Those are the minimum of energy that corresponds to the IC value of the modulation parameter and the equality of energies of the perturbed and non-perturbed states that corresponds to multiplication of the unit cell (the ratio is equal to 2). Considering the energy states as the prototypes of bands, normalized by the perturbation, one can come to conclusion that the distance between them (i.e., the bandgap width) might change its value with changing modulation period.

The results of analysis of the band splitting due to the IC superlattices will be reported in a forthcoming paper.

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